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Magnetic Correlations in the Hubbard Model on Triangular and Kagomé Lattices

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In order to study the magnetic properties of frustrated metallic systems, we present, for the first time, quantum Monte Carlo data on the magnetic susceptibility of the Hubbard model on triangular and kagomé lattices. We show that the underlying lattice structure determines the nature and the doping dependence of the magnetic fluctuations. In particular, in the doped kagomé case we find strong short-range magnetic correlations, which makes the metallic kagomé systems a promising field for studies of superconductivity.

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Frustrated spin systems have received significant attention because of the possibility of novel magnetic ground states and excitations [1]. The triangular spin-1/2 Heisenberg model has long-range magnetic order in the ground state, while the spin-1/2 Heisenberg model on the kagomé lattice is considered to be disordered. The discovery of superconductivity at 5 K in $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ has generated new interest in frustrated interacting systems [2]. Furthermore, superconductivity has been recently discovered in β -pyrochlore osmate KOs_2O_6 with a T_c of 10 K [3]. This generates further interest in the magnetic properties of frustrated interacting systems.

In cobaltates, cobalt and oxygen ions form a two-dimensional triangular network. The hopping matrix element of electrons in the cobalt 3d orbitals is not isotropic, and it has been shown that the triangular CoO_2 lattice consists of four coupled kagomé sublattices [4]. Hence, it is important to compare the magnetic properties of interacting systems on triangular and kagomé lattices. The electronic properties of the t - J and the Hubbard models on the triangular and kagomé lattices have been studied using various techniques of many-body physics. The triangular t - J model was investigated within the resonating-valence-bond framework [5–7] and by using high-temperature expansions [8]. The triangular Hubbard model was studied with the path-integral renormalization-group (RG) [9], the one-loop RG [10], and the fluctuation-exchange (FLEX) [11] approaches. The FLEX method was also used for studying the magnetic properties of the Hubbard model on the kagomé lattice [12].

In this Letter, we compare the nature of the magnetic correlations in the Hubbard model on the triangular and the kagomé lattices using quantum Monte Carlo (QMC) simulations. We consider the Hubbard model on the kagomé lattice to be a simple limiting case to explore for new physics due to the underlying orbital structure in frustrated interacting systems. The orbital degrees of freedom create the possibility for mixing the spin and charge channels, and hence of new electronic states. This is important because of the general ongoing research effort on the transition metal oxides. These are our motivations for performing the QMC

calculations on the Hubbard model on the triangular and the kagomé lattices. We are particularly interested in the doped cases of these models for which there are no exact calculations on the magnetic properties.

In the following, we will see that the triangular Hubbard model has strong antiferromagnetic (AFM) correlations near half filling and at low temperatures, when the Coulomb repulsion U is of the order of the bandwidth. On the other hand, for weak U , the magnetic correlations saturate as $T \rightarrow 0$. In the kagomé lattice, the unit cell consists of three atoms and the unit cells form a triangular lattice, as seen in Fig. 1(a). Consequently, there are three bands of magnetic excitations. Two of these modes involve enhanced short-range AFM correlations. In particular, we find that in the doped kagomé case the low-frequency short-range AFM correlations are stronger in comparison to the triangular lattice. Hence, it would be useful to investigate the possibility of superconductivity in metallic kagomé systems. We think that the results presented here will be useful for understanding the magnetic properties of frustrated interacting systems.

The Hubbard model is defined by

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}, \quad (1)$$

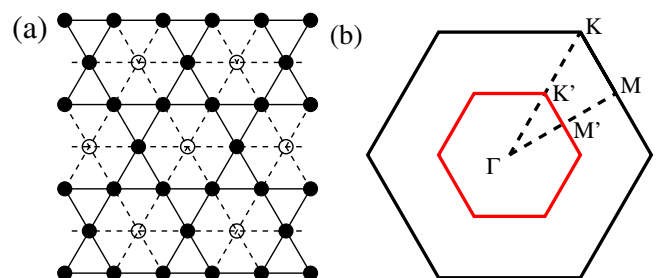


FIG. 1 (color online). (a) Sketch of the triangular and the kagomé lattices. The kagomé lattice is obtained from the triangular lattice by removing the sites with the open circles. (b) First Brillouin zones of the triangular (black) and the kagomé (red) lattices.

where t is the hopping matrix element between the nearest-neighbor sites, U is the on-site Coulomb repulsion, and μ is the chemical potential. Here, $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) annihilates (creates) an electron with spin σ at site i , and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. In the following, we will take $t < 0$ and consider $\langle n \rangle \geq 1.0$, which is the appropriate case for the cobaltates [4]. In obtaining the data presented here, the determinantal QMC technique [13] was used. At low T , this technique has the sign problem [14] for the triangular and kagomé lattices even at half filling, due to the absence of the particle-hole symmetry. Because of the sign problem, we have used a parallel computer to obtain the QMC data presented here.

For the triangular lattice, the magnetic susceptibility at frequency $\omega = 0$ is defined by

$$\chi(\mathbf{q}) = \int_0^\beta d\tau \sum_{\ell} e^{-i\mathbf{q} \cdot \mathbf{r}_\ell} \langle m^z(\mathbf{r}_{i+\ell}, \tau) m^z(\mathbf{r}_i) \rangle, \quad (2)$$

where $m^z(\mathbf{r}_i) = c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}$ and $m^z(\mathbf{r}_i, \tau) = e^{H\tau} m^z(\mathbf{r}_i) e^{-H\tau}$. Here, χ will be plotted in units of $|t|^{-1}$.

The kagomé lattice is a three-band model, since each unit cell consists of three sites. Hence, each lattice site on the kagomé lattice can be represented by the indices (l, d) where l is the unit-cell index and d denotes the atomic site in a particular unit cell. The corresponding Brillouin zone (BZ) is reduced with respect to the triangular case as illustrated in Fig. 1(b). For the kagomé case, we define the magnetic susceptibility at $\omega = 0$ as

$$\chi_{dd'}(\mathbf{q}) = \int_0^\beta d\tau \sum_{\ell} e^{-i\mathbf{q} \cdot \mathbf{r}_\ell} \langle m_d^z(\mathbf{r}_{i+\ell}, \tau) m_{d'}^z(\mathbf{r}_i) \rangle, \quad (3)$$

where $m_d^z(\mathbf{r}_i) = c_{id\uparrow}^\dagger c_{id\uparrow} - c_{id\downarrow}^\dagger c_{id\downarrow}$, $c_{id\sigma}$ ($c_{id\sigma}^\dagger$) is the annihilation (creation) operator of an electron with spin σ at lattice site (i, d) . Diagonalizing the 3×3 matrix $\chi_{dd'}(\mathbf{q})$, we obtain $\chi_\alpha(\mathbf{q})$, which describes the kagomé magnetic bands. We also note that already for the noninteracting ($U = 0$) case, the triangular and the kagomé lattices have different properties. For $t < 0$, the one-electron density of states $N(\omega)$ of the triangular lattice has a van Hove singularity at $\langle n \rangle = 0.5$. For the kagomé lattice, there is a δ -function singularity in $N(\omega)$ at the bottom of the band and there are van Hove singularities at $\langle n \rangle = 1.16$ and 1.51 . In addition, $N(\omega = 0)$ vanishes at $\langle n \rangle = 1.33$. These features of $N(\omega)$ are also reflected in the magnetic susceptibilities of the noninteracting case.

We first present results for the triangular lattice at half filling. Figure 2(a) shows $\chi(\mathbf{q})$ versus \mathbf{q} for $U = 4|t|$ on various size lattices as the temperature is lowered. Here, it is seen that $\chi(\mathbf{q})$ has a broad peak centered at the K point of the BZ. We also note that $\chi(\mathbf{q})$ does not vary significantly at low T . For comparison, $\chi_0(\mathbf{q})$ for the noninteracting system at $T = 0.17|t|$ is shown by the dotted curve. Figure 2(b) displays $\chi(\mathbf{q})$ versus \mathbf{q} for $U = 8|t|$ at half filling, where we observe a large Stoner enhancement of the AFM correlations. In contrast with the $U = 4|t|$ case,

here, $\chi(\mathbf{q})$ at the K point grows rapidly with a Curie-like T dependence, as T decreases from $1|t|$ to $0.33|t|$. However, it is not known whether $\chi(\mathbf{q})$ saturates at lower T for $U = 8|t|$. These results show that the T dependence of $\chi(\mathbf{q})$ depends strongly on the value of $U/|t|$ in the triangular Hubbard model, in agreement with the findings of the path-integral RG calculations [9].

Figure 2(c) shows the filling dependence of $\chi(\mathbf{q})$ for $U = 8|t|$ and $T = 0.33|t|$. Here, we observe that the AFM correlations decay monotonically as the electron filling is varied from 1.0 to 1.3. We have also performed calculations for $\chi(\mathbf{q})$ at higher electron fillings. We find that, when $\langle n \rangle$ is increased to 1.5, the peak in $\chi(\mathbf{q})$ shifts to the M point. Upon further doping to $\langle n \rangle = 1.75$, we find that, for $U = 8|t|$ and $T = 0.2|t|$, the Stoner enhancement is about 20%. Hence, for this dilute hole concentration, the magnetic correlations are weakly affected by the presence of the on-site U at this temperature.

Next, we discuss the magnetic properties of the Hubbard model on the kagomé lattice. Figure 3(a) shows QMC

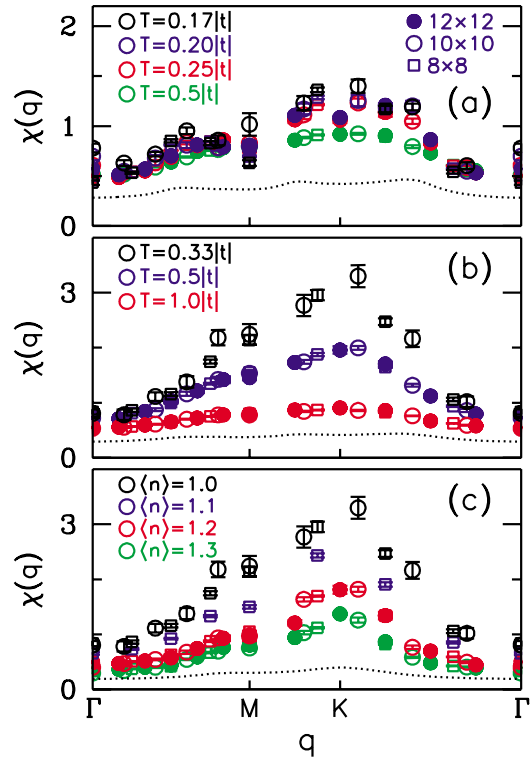


FIG. 2 (color online). Magnetic susceptibility $\chi(\mathbf{q})$ versus \mathbf{q} of the triangular Hubbard model at zero frequency. Here, \mathbf{q} is scanned along the path $\Gamma \rightarrow M \rightarrow K \rightarrow \Gamma$ in the BZ of the triangular lattice illustrated in Fig. 1(b). The temperature evolution of $\chi(\mathbf{q})$ at half filling is shown in (a) for $U = 4|t|$ and in (b) for $U = 8|t|$. In these figures, the dotted curves represent results for the noninteracting case at the lowest temperature used in that figure. The evolution of $\chi(\mathbf{q})$ versus \mathbf{q} with the electron density $\langle n \rangle$ is shown in (c) for $U = 8|t|$ and $T = 0.33|t|$. Here, the dotted curve represents the results for the noninteracting system at $\langle n \rangle = 1.3$ and $T = 0.33|t|$.

results on $\chi_\alpha(\mathbf{q})$ for $U = 4|t|$ and $T = 0.2|t|$ at half filling. Here, $\chi_\alpha(\mathbf{q})$ for the three magnetic bands are plotted as a function of \mathbf{q} , and the red curves represent results for the noninteracting case. In this figure, we observe that the top band ($\alpha = 1$) is flat in \mathbf{q} space, and the second magnetic band ($\alpha = 2$) is degenerate with the first one at the zone center. The third mode is weaker in magnitude and exhibits a smooth \mathbf{q} dependence. Figure 3(b) shows $\chi_\alpha(\mathbf{q})$ versus \mathbf{q} for $U = 8|t|$ and $T = 0.33|t|$ at half filling. The general features are similar to those seen in Fig. 3(a), however, here the Stoner enhancement is larger. In Fig. 3(c), the QMC results are shown for $U = 4|t|$ and $T = 0.14|t|$ at $\langle n \rangle = 1.15$. These figures show that the features of $\chi_\alpha(\mathbf{q})$ are in correspondence with those of the noninteracting case.

We note that the kagomé lattice is obtained from the triangular lattice, as illustrated in Fig. 1(a), by removing the sites with the empty circles. This is equivalent to putting an infinitely repulsive one-electron potential at these sites. Bragg scattering from this static charge-density-wave field then folds the BZ of the triangular lattice, and also mixes the different wave vector components of the

spin fluctuations. It is this process which creates the kagomé magnetic bands.

We next discuss the T dependence of the magnetic correlations in the kagomé lattice. Figure 4(a) shows $\chi_1(\mathbf{q} = 0)$ versus T for $U = 4|t|$ and $8|t|$ at $\langle n \rangle = 1.0$ and 1.15 . Here, we observe that, at half filling and for $U = 4|t|$, $\chi_1(\mathbf{q} = 0)$ saturates as T decreases. On the other hand, for $U = 8|t|$, $\chi_1(\mathbf{q} = 0)$ has a strong T dependence. For $\langle n \rangle = 1.15$ and $U = 4|t|$, we observe that $\chi_1(\mathbf{q} = 0)$ gets enhanced at low T , and becomes larger than at half filling. We also see that the enhancement of $\chi_1(\mathbf{q} = 0)$ depends on the lattice size. However, this type of nonmonotonic doping dependence was not observed for the triangular Hubbard model. In addition, we observe that, for $U = 8|t|$ and at half filling, $\chi_1(\mathbf{q} = 0)$ exhibits a Curie-like T dependence for $0.25|t| \leq T \leq 1.0|t|$. In the ground state of the Heisenberg model on the kagomé lattice, it is considered that a spin gap $\Delta_S \approx J/20$ exists, where J is the magnetic exchange [1]. For $U = 8|t|$, we have $J \approx 4t^2/U = 0.5|t|$, which gives $\Delta_S \approx 0.025|t|$. We expect that $\chi_\alpha(\mathbf{q})$ saturates before T becomes comparable to Δ_S .

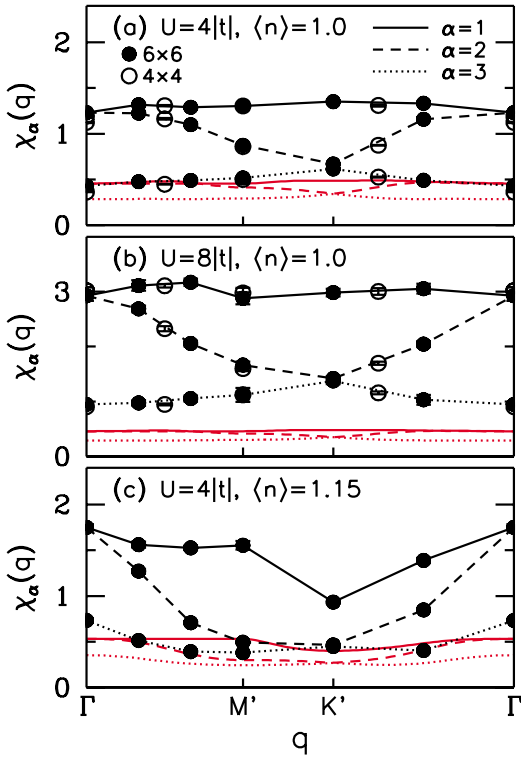


FIG. 3 (color online). Magnetic susceptibility $\chi_\alpha(\mathbf{q})$ versus \mathbf{q} for the Hubbard model on the kagomé lattice at zero frequency. Here, the three magnetic modes of $\chi_\alpha(\mathbf{q})$ are shown at each \mathbf{q} point, as \mathbf{q} is scanned along the path $\Gamma \rightarrow M' \rightarrow K' \rightarrow \Gamma$ in the first BZ of the kagomé lattice. Results on $\chi_\alpha(\mathbf{q})$ at half filling are shown in (a) for $U = 4|t|$ and $T = 0.2|t|$ and in (b) for $U = 8|t|$ and $T = 0.33|t|$. These data have been obtained on lattices with 6×6 and 4×4 unit cells. In (c), results are shown for $\langle n \rangle = 1.15$ with $U = 4|t|$ and $T = 0.14|t|$. In these figures, the data points for the 6×6 lattice are connected by black lines, and the red curves represent the results for the noninteracting case.

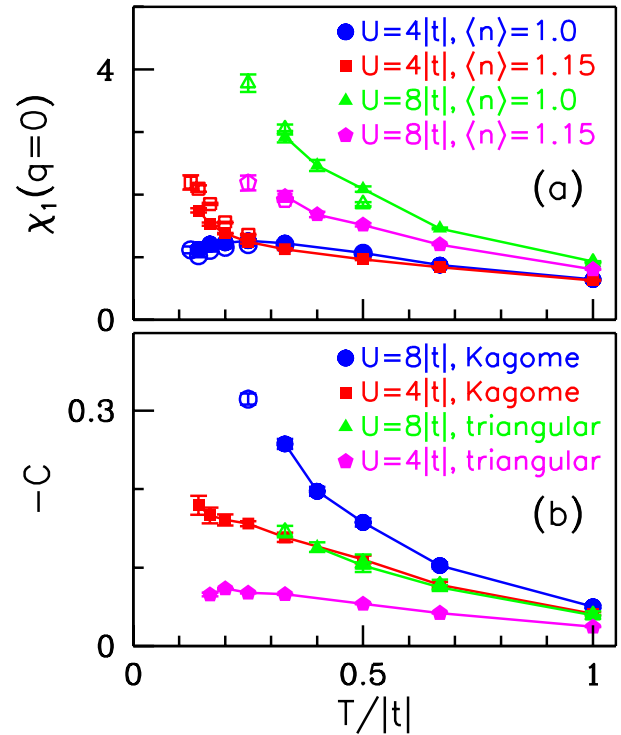


FIG. 4 (color online). (a) $\chi_1(\mathbf{q} = 0)$ versus T for the kagomé lattice with $U = 4|t|$ and $8|t|$ at $\langle n \rangle = 1.0$ and 1.15 . (b) Zero-frequency component of the magnetic correlations between the nearest-neighbor sites C versus T for the kagomé and the triangular lattices at $\langle n \rangle = 1.15$ for $U = 8|t|$ and $4|t|$. In these figures, the results on the kagomé lattice were obtained for 6×6 (filled points) and 4×4 (empty points) unit cells, and the results on the triangular lattice are for 12×12 (filled points) and 8×8 (empty points) lattices. In addition, the data points for the 6×6 kagomé and the 12×12 triangular lattices have been connected by solid lines.

The FLEX calculations for the Hubbard model on the kagomé lattice find that the leading magnetic mode is nearly \mathbf{q} independent, and the tendency to electronic instabilities is suppressed [12]. We note that while the $\alpha = 1$ mode is nearly \mathbf{q} independent, the $\alpha = 2$ mode has ferromagnetic \mathbf{q} dependence in the sense that it decreases away from the Γ point. In addition, the eigenvectors of $\chi_{dd}(\mathbf{q})$ show that, at $\mathbf{q} \approx 0$, the $\alpha = 1$ and 2 modes describe excitations involving the AFM polarization of the spins within a unit cell [15]. Away from $\mathbf{q} = 0$, these modes have additional structures, however they involve AFM polarizations over most of the BZ. Hence, these two modes contain enhanced short-range AFM fluctuations. Within the context of superconductivity mediated by magnetic fluctuations, a relevant quantity is the zero-frequency component of the magnetic fluctuations between the two nearest-neighbor sites i and j ,

$$C = \int_0^\beta d\tau \langle m^z(\mathbf{r}_i, \tau) m^z(\mathbf{r}_j) \rangle. \quad (4)$$

In Fig. 4(b), we compare C versus T for the triangular and the kagomé lattices for $U = 4|t|$ and $8|t|$ at $\langle n \rangle = 1.15$. This figure shows that, at these temperatures, the nearest-neighbor AFM correlations are stronger for the kagomé lattice, even though the ground state of the spin-1/2 Heisenberg model has long-range order on the triangular lattice and it is disordered in the kagomé case. Hence, it would be useful to investigate the possibility of superconductivity in metallic kagomé systems.

Finally, we discuss the implications of these data for the magnetic correlations observed in the cobaltates. The cobaltates have a rich phase diagram with superconductivity found for $x \approx 0.35$ in $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ [2] and with magnetic order and large quasiparticle renormalizations observed in Na_xCoO_2 when x is near 0.75 [16]. For the triangular Hubbard model, we find that the magnetic correlations are strongest at half filling, and the correlation effects are weak in the overdoped regime $\langle n \rangle \geq 1.5$. In contrast, for the kagomé lattice we have seen that the magnetic correlations can be stronger in the doped case when $U = 4|t|$. However, in both of these models, we find that the correlation effects are most prominent in the vicinity of half filling at the temperatures where the QMC calculations were performed. We note that it would be useful to determine experimentally the \mathbf{q} dependence of the magnetic fluctuations in the superconducting $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$.

In this Letter, we have presented exact numerical results on the magnetic correlations in the Hubbard model on the triangular and kagomé lattices. At the temperatures where the QMC calculations were performed, we find, in both of these models, that the magnetic correlations grow rapidly as T decreases at half filling for $U = 8|t|$, while they saturate when $U = 4|t|$. In the triangular Hubbard model, the AFM correlations decay monotonically with the elec-

tron doping. In the kagomé case, on the other hand, we have seen that the magnetic correlations can be stronger in the doped case when $U = 4|t|$. We have also seen that in the kagomé case the BZ is reduced and there are three modes of magnetic excitations. The two leading modes involve short-range AFM correlations. In particular, we find that the low-frequency short-range AFM correlations are stronger in the doped kagomé case than in the triangular case. This makes the interacting metallic systems with kagomé type lattice structures a promising field for studies of superconductivity. We think that these results will be useful for understanding the magnetic properties of frustrated interacting systems.

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